

Evidence for the droplet/scaling picture of spin glasses

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We have studied the Parisi overlap distribution for the three-dimensional Ising spin glass in the Migdal-Kadanoff approximation. For temperatures $T \simeq 0.7T_c$ and system sizes up to $L = 32$, we found a $P(q)$ as expected for full Parisi replica symmetry breaking, just as was also observed in recent Monte Carlo simulations on a cubic lattice. However, for lower temperatures our data agree with predictions from the droplet or scaling picture. The failure to see droplet model behavior in Monte Carlo simulations is due to the fact that all existing simulations have been done at temperatures too close to the transition temperature so that system sizes larger than the correlation length have not been achieved.

Despite over two decades of work, the nature of the low-temperature phase of the three-dimensional Edwards-Anderson spin glass remains controversial. While the best available computer simulation results to date [1–3] have been interpreted as suggesting a mean-field like behavior with replica-symmetry breaking (RSB) and a variety of different pure states [4], analytical arguments [5] favor a droplet picture [6–8], in which there are only a single pair of spin-flip related pure states. It is the purpose of this paper to present evidence that the apparent RSB observed in Monte Carlo simulations is due to the relatively small system sizes used and the proximity of the simulational temperature to T_c , so that these simulations merely probe the crossover region between the critical behavior and the true low-temperature behavior.

The droplet picture differs from mean-field theory most dramatically in the overlap distribution function

$$P(q, L) = \left\langle \left\langle \delta \left(q - \frac{\sum_{i=1}^N x_i S_i^{(1)} S_i^{(2)}}{\sum_{i=1}^N x_i} \right) \right\rangle \right\rangle. \quad (1)$$

Here, the superscripts (1) and (2) denote two replicas of the system, $N = L^3$ is the number of spins, and $\langle \dots \rangle$ and $[\dots]$ denote the thermodynamic and disorder average respectively. The coefficients x_i can be chosen in several ways, as discussed below. We use $P(q, L)$ to denote the overlap for a finite system of size L , reserving the more standard notation $P(q)$ to refer to the asymptotic form $\lim_{L \rightarrow \infty} P(q, L)$.

In the mean-field RSB picture, $P(0)$ is finite in the spin-glass phase, while it is zero in the droplet picture. The main support for the mean-field picture comes from the observation that $P(0, L)$ does not decrease with increasing system size in systems up to size $N = L^3 = 16^3$ at temperatures as low as $0.7T_c$. However (and this is the main motivation for our work), even within the droplet picture one expects to see a stationary $P(0, L)$ for a certain range of system sizes and temperatures. The reason is that at T_c the overlap distribution $P(q, L)$ obeys the scaling law

$$P(q, L) = L^{\beta/\nu} \tilde{P}(qL^{\beta/\nu}), \quad (2)$$

β being the order parameter critical exponent, and ν the correlation length exponent. In $d = 3$, $\beta/\nu \simeq 0.3$ [3], implying that the critical $P(0, L)$ increases with L . On the other hand, in $d = 3$, the droplet picture predicts a decay

$$P(0, L) \sim 1/L^\theta$$

with an exponent $\theta \simeq 0.17$ when L is larger than the (temperature-dependent) correlation length. Thus, for temperatures not too far below T_c , one can expect an almost stationary $P(0, L)$ for a certain range of system sizes. Since both β/ν and θ are rather small, this apparent stationarity may persist over a considerable range of system sizes L . We will argue that this is the correct interpretation of the simulation data at $T \simeq 0.7T_c$ reported in [1]. This possibility was discussed in [9] where the authors studied the four dimensional EA spin glass by Monte Carlo simulations. However, they concluded that their Monte Carlo data could not be interpreted in these terms. We will comment on their work at the end of this paper.

In the following, we will study the overlap distribution for the three-dimensional Edwards-Anderson spin glass in the MK approximation. Compared to Monte Carlo simulations, the MK approximation has the advantage that system sizes up to $L = 32$ and temperatures down to $0.2T_c$ can be investigated with only a few days' CPU time. Since the MK approximation has proven to give good results for the phase diagram and the critical exponents of the three-dimensional spin glass [10], we expect that it will also capture the main features of the overlap distribution. Furthermore, it was shown analytically in [11] that in infinite dimensions (and in an expansion away from infinite dimensions) the MK approximation gives

$$P(q) = (1/2)(\delta(q + q_{EA}) + \delta(q - q_{EA})), \quad (3)$$

just as is expected in the droplet picture. In the present paper we shall investigate the role of finite size effects on the overlap distribution function, i.e., $P(q, L)$ for a commonly used Ising spin glass model.

The Edwards-Anderson spin glass in the absence of an external magnetic field is defined by the Hamiltonian

$$H = - \sum_{\langle i, j \rangle} J_{ij} S_i S_j,$$

where the Ising spins can take the values ± 1 , and the nearest-neighbor couplings J_{ij} are independent from each other and Gaussian distributed with a standard deviation J . Evaluating a thermodynamic quantity in MK approximation in three dimensions is equivalent to evaluating it on an hierarchical lattice that is constructed iteratively by replacing each bond by eight bonds, as indicated in Fig. 1. The total number of bonds after I iterations is 8^I , which is identical to the number of lattice sites of a three-dimensional lattice of size $L = 2^I$. Thermodynamic quantities are then evaluated iteratively by tracing over the spins on the highest level of the hierarchy, until the lowest level is reached and the trace over the remaining two spins is calculated [10]. This procedure generates new effective couplings, which have to be included in the recursion relations.



FIG. 1. Construction of a hierarchical lattice.

The coefficients x_i in Eq. (1) are often chosen to be equal to 1 for all i . In fact, for a cubic lattice this is the most natural choice since all the spins then have the same coefficients. However, on a hierarchical lattice where not all spins are equivalent, the more natural choice is one which ensures that all the bonds occur with the same coefficient, i.e.,

$$\frac{\sum_{i=1}^N x_i S_i^{(1)} S_i^{(2)}}{\sum_{i=1}^N x_i} = \sum_{\langle ij \rangle} \frac{S_i^{(1)} S_i^{(2)} + S_j^{(1)} S_j^{(2)}}{2N_L} \quad (4)$$

where $\langle ij \rangle$ is a sum over all bonds [11] and N_L is the number of bonds. Our numerical results presented below are for this second choice, but we have found very similar results for the first choice of x_i .

It is possible to calculate $P(q, L)$ directly from the above definition Eq. (1). However, it is more expedient to first calculate the Fourier transform $F(y, L)$ of $P(q, L)$, which with the choice of Eq. (4) is given by [11]

$$F(y, L) = \left\langle \exp \left[i y \sum_{\langle ij \rangle} \frac{(S_i^{(1)} S_i^{(2)} + S_j^{(1)} S_j^{(2)})}{2N_L} \right] \right\rangle. \quad (5)$$

The recursion relations for $F(y, L)$ involve two- and four-spin terms, and can easily be evaluated numerically. The

Parisi overlap distribution is a sum of a large number of delta function terms corresponding to the possible projections of the spins in one replica onto the spins in the second replica i.e.

$$P(q) = \sum_{n=-N_L/2}^{N_L/2} a_n \delta(q - 2n/N_L). \quad (6)$$

The coefficients a_n can be evaluated from $F(y, L)$:

$$a_n = (2/\pi N_L) \int_0^{\pi N_L/2} F(y, L) \cos(2yn/N_L) dy. \quad (7)$$

Our numerical results are illustrated in the next five figures. In all simulations we made sure that the range and number of y values, as well as the number of samples, were sufficiently large to give reliable results. Fig. 2 shows $P(q, L)$ for 2, 3, 4, and 5 iterations, averaged over up to 10000 realizations of randomness, and for $T = 0.7T_c$, where $T_c \approx 0.88J$ [10]. We have displayed the $P(q, L)$ as smooth curves, rather than as a large number of delta function spikes for ease of viewing. These curves correspond to system sizes $L = 4, 8, 16, 32$. Since $P(q, L) = P(-q, L)$, the curves are only shown for positive q values. Just as in the Monte Carlo simulations of [1–3], the value of $P(0, L)$ and the area under the main peak hardly change with L , a result which is compatible with the RSB picture.

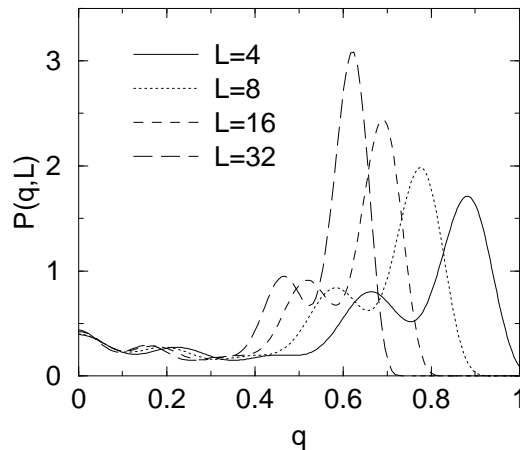


FIG. 2. $P(q, L)$ at $T \simeq 0.7T_c$, averaged over 5000-10000 bond realizations of the randomness

In contrast to the Monte Carlo simulations, our $P(q, L)$ has not only two large peaks, but also seven smaller equidistant peaks, or bumps. This indicates that certain overlap values occur more often than their neighboring values and arises from the hierarchical structure of the lattice: the 6 spins that are traced over last, have the highest coordination number, and the 8 “bubbles” sitting between those spins are to some degree slaved to the state of these spins. If we assume that each “bubble” has two

flip-related states, we find 9 equidistant preferred values for the overlap. For MK approximation in two dimensions, the same argument gives 5 preferred values, and 17 in four dimensions. We have confirmed these predictions by calculating $P(q, L)$ in 4 and 2 dimensions. In two dimensions, we chose a ferromagnet, in order to make sure that the bumps are independent of the spin-glass properties. As will be seen from our low-temperature data, only the peak at q_{EA} survives in the thermodynamic limit.

We now discuss the remaining part of our results. In Fig. 7 of [1] the authors plotted the overlap distribution for a single sample of a cubic Ising spin glass, i.e., without averaging over the disorder. These distributions have in general several peaks and look very different for different samples, just as they would in the presence of RSB. Fig. 3 shows our equivalent result for four randomly chosen samples at $T = 0.7T_c$ and $L = 32$. The good agreement with the Monte Carlo data shows again that the MK approximation reproduces one of the main features of the three-dimensional spin glass simulations. Incidentally, it is this large sample to sample variation which requires one to average over very large number of bond realizations of the randomness to get smooth averaged expressions for $P(q, L)$.

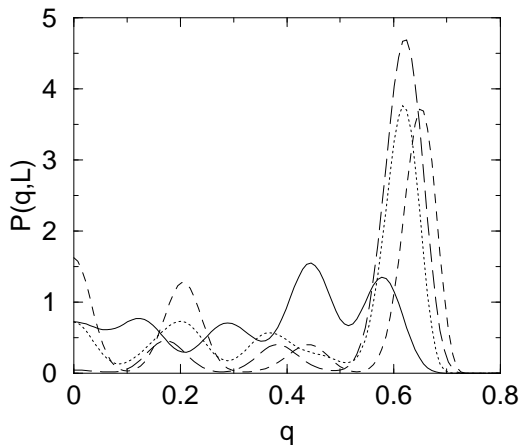


FIG. 3. The overlap distribution for four different bond realizations, at $T = 0.7T_c$ and $L = 32$.

While numerical data at temperatures around $T = 0.7T_c$ are compatible with RSB, data for lower temperatures are in favor of the simpler droplet picture. For $T = 0.38T_c$, e.g., $P(q, L)$ decreases with increasing system size for small values of q , the area under the subsidiary bumps decreases, and the area under the main peak increases, as shown in Fig. 4.

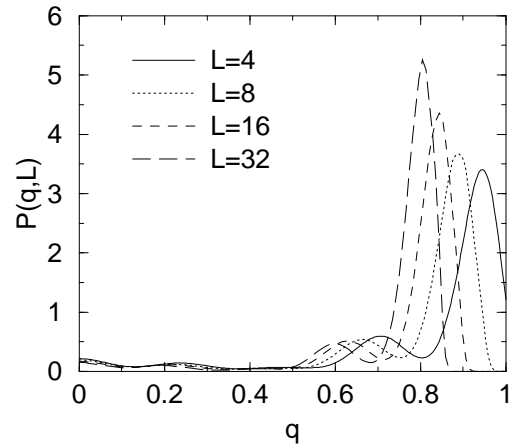


FIG. 4. $P(q, L)$ at $T \simeq 0.38T_c$, averaged over 5000-10000 bond realizations.

In order to make these qualitative statements more quantitative, we have evaluated $P(0, L)$ for a variety of temperatures and system sizes, each point again being averaged over 5000-25000 samples (Fig. 5).

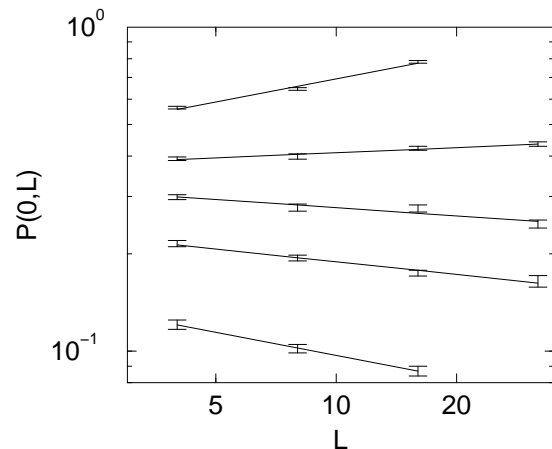


FIG. 5. The value of $P(0, L)$, and its standard error, as function of the system size, for $T/T_c = 1, 0.7, 0.54, 0.38, 0.2$ (from top to bottom). The straight lines are power-law fits with the exponents 0.24, 0.053, -0.084, -0.13, -0.24 (from high to low temperatures).

One can clearly see that for lower temperatures $P(0, L)$ decreases with increasing system size, without any indication of a saturation at a nonzero value. For the lowest simulated temperature, the decrease is characterized by the exponent θ , as predicted by the droplet picture. (In [10,12], $\theta \simeq 0.26$ is found in MK approximation.) On the other hand, the data at T_c are compatible with the exponent $\beta/\nu \simeq 0.26$ obtained earlier [10]. The data sets for intermediate temperatures each cover a small window of less than one decade in the system size L in the crossover region between the two limiting regimes. With this small range of L -values, one does not see the crossover expected at larger system sizes to a line with the slope $-\theta$. But

one sees an effective exponent in the range before this asymptotic behavior sets in. Because the behavior is so well described by an effective exponent, it is not possible to obtain a reliable estimate of the correlation length. The only statement one can make is that for temperatures above $0.38T_c$ the correlation length would seem to be (much) greater than 32 lattice spacings. This seems to rule out any possibility of achieving a satisfactory simulation of the three dimensional spin glass phase with current computers and algorithms. (Simulations at low temperature, where the correlation length is certainly small, are very hard as the spins are almost totally frozen up on typical simulational timescales).

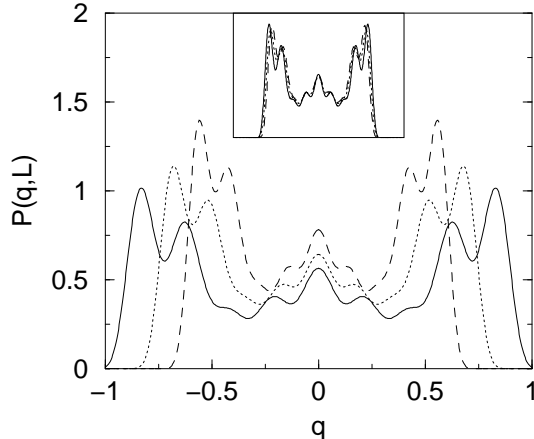


FIG. 6. The overlap distribution at $T = T_c$, for $L = 4$ (solid), 8 (dotted), 16 (dashed). The inset shows a scaling collapse $P(q, L)/L^{0.24}$ vs $qL^{0.24}$.

The simulational data [1,2] is also purported to provide evidence for a non-trivial ultrametric topology amongst the alleged multiplicity of pure states. However, it has been known for many years that such behavior can again be an artifact of finite size effects when the correlation length becomes comparable with the linear dimension of the system [13].

Finally we comment on results in four dimensions. While it is suggested in [5] that the mean-field RSB picture cannot hold in any finite dimension, Monte Carlo data for temperatures $T \simeq 0.67T_c$ show a saturation of $P(0, L)$ for system sizes up to $L = 6$, after an initial decline for sizes $L = 2$ and 3 [9]. It is quite possible that the Monte Carlo data for $L = 2, 3$ cannot really be trusted and the decrease seen by these authors is attributable to some finite size effects. In fact, it has been noted in other studies that $P(q, L = 2)$ does not scale well close to criticality [14]. We studied the four dimensional problem briefly within the MK scheme. We will not display our data here, but simply state that they also show a stationary $P(0, L)$ at $T \simeq 0.67T_c$ for 2 and 3 iterations, i.e. for $L = 4$ and $L = 8$. However, at $T \simeq 0.33T_c$, we see a clear decline in $P(0, L)$ when going from $L = 4$

to $L = 8$. This indicates that at $T \simeq 0.67T_c$, the system is not yet in the asymptotic regime for system sizes $L \leq 8$. However, since the exponents β/ν and θ are much larger in four dimensions than in three dimensions, the change in the slope of $\ln P(0, L)$ vs $\ln L$ must be faster in four dimensions than in three dimensions. Therefore, if one goes to somewhat larger system sizes than in [9], it might actually be possible to escape the effects of critical fluctuations and see features characteristic of the low-temperature phase proper, in contrast to the situation in three dimensions, where escape from critical fluctuation effects seems impossible.

In summary, the MK approximation gives clear evidence that the apparent RSB behavior of the three-dimensional Edwards-Anderson spin glass reported in [1–3] is due to finite size effects arising from the closeness of the temperatures studied to the critical temperature T_c so that the correlation length is larger than the linear dimension of the systems studied.

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